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ABSTRACT

The electrical conductivity of n-type InSb in the temperature range 77K - 300K has been calculated by using the Boltzmann equation with a relaxation time ansatz. The two dominant scattering mechanisms in this temperature range are the impurity scattering and the polar scattering. The hydrostatic pressure effects on the electrical conductivity have been studied by considering the variations of the band structure, the carrier concentration, the electron effective mass and the static dielectric constant of the material. The variation of the electrical conductivity up to 10 kbar at the temperatures T = 81 K and T = 290 K is compared with experimental data.

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TABLE OF CONTENTS

Introduction

The transport properties of InSb at atmospheric pressure have been widely studied theoretically in the last two decades.[1-5] Although it is experimentally well known that the energy differences between the various band extrema of this material are pressure sensitive[6,7] and consequently the electrical conductivity is strongly pressure dependent, there is no systematic calculation so far to explain the hydrostatic pressure effect on the electrical conductivity. It is the purpose of the present work to present a calculation for the pressure dependent electrical conductivity in two characteristic temperature ranges, 77 K to 100 K and 200 K to 300 K.

Kane calculated the band structure of InSb using the $\underset{\sim}{k} \cdot \underset{\sim}{p}$ perturbation approach and showed that the isoenergetic surfaces of the first conduction band (as well as that of the light-hole valence band) are spherically symmetric while the dispersion relations between energy and wave number are nonparabolic.[8] In Chapter 1, we shall briefly derive various expressions for the electrical conductivity at different temperatures using the Boltzmann equation approach with a conventional relaxation time ansatz, but considering explicitly the specific nature of the energy band structure of InSb. The dominant scattering mechanisms in the two different temperature ranges are assumed to be

the impurity scattering (77 K - 100 K) and the polar scattering (200 K - 300 K).

The main effect of the hydrostatic pressure on InSb is the variation of the energy differences between the various band extrema. In the electrical conductivity expressions, the pressure dependent parameters are the carrier concentration, the electron effective mass, the static dielectric constant and the generalized Fermi-Dirac integrals which are used to describe properly the nonparabolic band structure. In Chapter 2, we study the dependence of these parameters on the energy differences between the various band extrema, and hence on pressure.

In the last two chapters, we apply the results of the previous chapters to calculate the pressure dependent electrical conductivity of n-InSb up to 10 kbar at 81 K and 290 K. The calculated results are compared with the presently available experimental results.[9] In general, the theory is in good agreement with the experiment in the low pressure range (0 kbar - 5 kbar), and progressive divergence from the experimental results occurs for higher pressures. Possible reasons for the disagreement are discussed.

CHPATER 1 The Electrical Conductivity of InSb

The electrical conductivity is defined as the current density per unit external electric field applied to the conducting material. In this chapter, we make a comparably simple calculation to derive the electrical conductivity of n-InSb in the temperature range from 77 K to 300 K by assuming a relaxation time τ exists and also by considering the proper description of the conduction energy band of InSb. It is known that the energy in the first conduction band of InSb is spherically symmetric but the relation between the energy and the wave number k is not quadratic (i.e. nonparabolic).[8]

1.1 The Electrical Conductivity for Semiconductor with Spherical Energy Surfaces

The current density is defined as

$$\underset{\sim}{J} = \frac{2}{(2\pi)^3} \int e \, \underset{\sim}{v}_k \, f_k \, d^3\underset{\sim}{k} \qquad (1.1)$$

where f_k is the distribution function of the carriers which is determined by the Boltzmann equation. Under the relaxation time ansatz, the Boltzmann equation is

$$\frac{\partial f_k}{\partial t} + \underset{\sim}{v}_k \cdot \frac{\partial f_k}{\partial \underset{\sim}{r}} + \frac{\underset{\sim}{F}}{m} \cdot \frac{\partial f_k}{\partial \underset{\sim}{v}_k} = - \frac{f_k - f_k^o}{\tau} \qquad (1.2)$$

where $\underset{\sim}{F}$ is the force on the carrier and f_k^o is the equilibrium distribution to which the carriers relax. Neglecting the temperature gradient within the sample and assuming the force $\underset{\sim}{F}$ arises solely due to an applied dc electric field $\underset{\sim}{E}$, we have

$$f_k - f_k^o = \left(- \frac{\partial f_k^o}{\partial E}\right) \tau \, \underset{\sim}{v}_k \cdot e\underset{\sim}{E} . \qquad (1.3)$$

By substituting (1.3) into (1.1), we obtain

$$\underset{\sim}{J} = \frac{e^2}{4\pi^3} \int \left(- \frac{\partial f_k^o}{\partial E}\right) \tau \, \underset{\sim}{v}_k \, (\underset{\sim}{v}_k \cdot \underset{\sim}{E}) \, d^3\underset{\sim}{k} . \qquad (1.4)$$

In InSb, the energy bands posses a spherical structure,[8] i.e. the bands in k-space are described by spherical energy surfaces,

$$E(\underset{\sim}{k}) = E\,(k) . \qquad (1.5)$$

This relation greatly simplifies the term $\underset{\sim}{v}_k \, (\underset{\sim}{v}_k \cdot \underset{\sim}{E})$ in (1.4) since the components of the velocity of the carriers $\underset{\sim}{v}_k$ become

$$v_{k_i} = \frac{1}{\hbar} \frac{\partial E(\underset{\sim}{k})}{\partial k_i}$$

$$= -\frac{1}{\hbar}\frac{dE(k)}{dk}\frac{\partial k}{\partial k_i}$$

$$= \frac{1}{\hbar k}\frac{dE(k)}{dk}k_i \qquad (1.6)$$

where k is the magnitude of the wave vector. For symbolic convenience, we define an effective mass m^*, which has been widely used in transport theory of semiconductors[10], by the relation

$$\frac{1}{m^*} \equiv \frac{1}{\hbar^2 k}\frac{dE}{dk} . \qquad (1.7)$$

Then the velocity components have the form

$$v_{k_i} = \frac{\hbar k_i}{m^*} . \qquad (1.8)$$

Assuming the electric field $\underset{\sim}{E}$ and the current density $\underset{\sim}{J}$ to be in the x-direction, we have

$$J_x = \sigma_{xx} E_x \equiv \sigma |\underset{\sim}{E}| ,$$

where the conductivity

$$\sigma = \frac{\hbar^2 e^2}{3\pi^2}\int_0^\infty \left(-\frac{\partial f_k^0}{\partial E}\right) \tau \left(\frac{1}{m^*}\right)^2 k^4 \, dk . \qquad (1.9)$$

1.2 The Nonparabolic Conduction Band in InSb

In order to evaluate the integral in (1.9), we need the band structure of the material under consideration. In InSb, the main contribution to the electrical conductivity is from the electrons in the first conduction band since the electron mobility of this band is very much larger than the hole mobilities of the various valence bands (although the light-hole mobility of the second valence band is comparable to that of the conduction electrons, the light-hole concentration is in fact so small that we can neglect its contribution to the conductivity).[11] Therefore we shall consider only the electrons in the first conduction band to contribute to the conductivity.

According to Kane's theory, the energy structure of the first conduction band in InSb is nonparabolic.[8] The conduction electron energy E_Γ as a function of electron wave number k is given by

$$E_\Gamma = \frac{\hbar^2 k^2}{2m_o} + \frac{1}{2}\left[-E_G^* + E_G^*\left(1 + \frac{8}{3}\frac{P^2k^2}{E_G^{*2}}\right)^{\frac{1}{2}}\right] \qquad (1.10)$$

where $2\pi\hbar$ is the Planck const., m_o is the rest mass of the electron, and P is the matrix element of the 'interband' interaction, a parameter to be determined by the experimental value of the effective mass m_Γ at the bottom of the conduction band. E_G^* is the effective

mass band gap which determines the curvature of the first conduction band (and thus determines the electron effective mass). E_G^* should be distinguished from the forbidden band gap E_G of the semiconductor.[1] We shall discuss the nature of these two quantities in the next chapter.

The square root term in (1.10) can be expanded in a power series provided that the condition

$$\frac{8}{3}\ \frac{P^2k^2}{E_G^{*2}} < 1$$

is valid. This requires that k be less than 0.138×10^7 cm^{-1} at a temperature T = 290 K which implies[3] an electron concentration of less than 1×10^{18} cm^{-3} -------- a condition readily met even at 290 K for the n-InSb samples containing up to 10^{17} cm^{-3} impurity donors.[11] Retaining terms up to k^4, we obtain

$$E_\Gamma = \frac{\hbar^2k^2}{2m_o} + \frac{2}{3}\ \frac{P^2k^2}{E_G^*} - \frac{4}{9}\ \frac{P^4k^4}{E_G^{*3}} \qquad (1.11)$$

Before we invert (1.11) to obtain the relation $k = k(E_\Gamma)$, it is useful to determine the matrix element P from the value of the effective mass m_Γ at the bottom of the first conduction band so that we can simplify the energy equation. The effective mass m_Γ^* of the energy band E_Γ is defined as[12]

$$\frac{1}{m_\Gamma^*} = \frac{1}{\hbar^2} \frac{\partial^2 E_\Gamma}{\partial k^2} \quad , \tag{1.12}$$

which with (1.11) may be written as

$$\frac{1}{m_\Gamma^*} = \frac{1}{m_o} + \frac{4}{3} \frac{P^2}{\hbar^2 E_G^*} - \frac{8}{3} \frac{P^4 k^2}{\hbar^2 E_G^{*3}} \tag{1.13}$$

Therefore at the bottom of the conduction band (k = 0), we have

$$\frac{1}{m_\Gamma} = \frac{1}{m_o} + \frac{4}{3} \frac{P^2}{\hbar^2 E_G^*} \quad , \tag{1.14}$$

and thus the value of P^2 can be determined from m_Γ by

$$P^2 = \frac{3}{4} \frac{\hbar^2 E_G^*}{m_\Gamma} (1 - \mu) \tag{1.15}$$

where we define the quantity μ as the ratio of the effective mass to the rest mass of the electron

$$\mu \equiv \frac{m_\Gamma}{m_o} \quad . \tag{1.16}$$

From experiment μ has a value of 0.013 at T = 2.2 K[13] and will change due to temperature and pressure arising from the change of the

effective mass band gap E_G^*.

Substitution of (1.15) into (1.11) gives

$$E_\Gamma = \frac{\hbar^2 k^2}{2m_o} + \frac{\hbar^2 k^2}{2m_\Gamma}(1 - \mu) - \tfrac{1}{4}\frac{(1 - \mu)^2}{m_\Gamma^2}\frac{\hbar^4 k^4}{E_G^*} . \quad (1.17)$$

The two solutions for k^2 in (1.17) are

$$k^2 = \frac{m_\Gamma E_G^*}{\hbar^2 (1 - \mu)^2}\left[1 \pm \sqrt{1 - 4(1 - \mu)^2 \frac{E_\Gamma}{E_G^*}}\right] . \quad (1.18)$$

We can expand the square root term in (1.18) in a power series provided that $4(1 - \mu)^2 E_\Gamma / E_G^* < 1$. This condition is again met for our sample of n-InSb which has 1×10^{14} cm^{-3} impurity donors. Making the expansion, we obtain

$$k^2 \simeq \frac{m_\Gamma E_G^*}{\hbar^2 (1 - \mu)^2}\left\{1 \pm \left[1 - 2(1 - \mu)^2 \frac{E_\Gamma}{E_G^*} - 2(1 - \mu)^4 \left(\frac{E_\Gamma}{E_G^*}\right)^2\right]\right\}$$

and thus for k, we have

$$k = \begin{cases} \pm \dfrac{\sqrt{2m_\Gamma E_G^*}}{\hbar(1-\mu)^2}\left[1 - (1-\mu)^2\,\dfrac{E_\Gamma}{E_G^*} - (1-\mu)^4\left(\dfrac{E_\Gamma}{E_G^*}\right)^2\right]^{1/2} & (1.19a) \\ \pm \dfrac{\sqrt{2m_\Gamma E_G^*}}{\hbar}\left[\dfrac{E_\Gamma}{E_G^*} + (1-\mu)^2\left(\dfrac{E_\Gamma}{E_G^*}\right)^2\right]^{1/2}. & (1.19b) \end{cases}$$

Since k is a slowly varying function of energy, having a finite value at zero energy, only (1.19b) satisfies the band structure of n-InSb. Furthermore, since μ is very small compared with unity, we can write

$$k = \frac{\sqrt{2m_\Gamma E_G^*}}{\hbar}\left[\frac{E_\Gamma}{E_G^*}\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^{1/2} \qquad (1.20)$$

Note that we choose the positive sign in (1.19b) which is required in obtaining a real physical description of transport properties of the conduction electrons. From (1.20), we also have

$$dk = \frac{\sqrt{2m_\Gamma E_G^*}}{2\hbar}\left[\frac{E_\Gamma}{E_G^*}\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^{-1/2}\left(1 + 2\,\frac{E_\Gamma}{E_G^*}\right) d\left(\frac{E_\Gamma}{E_G^*}\right). \qquad (1.21)$$

Relations (1.20) and (1.21) can be applied to obtain the electron concentration n_Γ in the first conduction band. The electron concentration is defined as

$$n = \int_{E_1}^{E_2} f_o(E)g(E)\, dE \tag{1.22}$$

where E_1 and E_2 are the upper and lower energies of the band, $f_0(E)$ is the Fermi-Dirac distribution and $g(E)dE$ is the density of states within an infinitesimal range of energy dE which can be expressed as

$$g(E)\, dE = \frac{1}{\pi^2} k^2 dk. \tag{1.23}$$

By substituting (1.20) and (1.21) into (1.22) and (1.23), we obtain

$$n_\Gamma = \frac{4}{\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2} \right)^{3/2} \int_0^\infty \frac{1}{1 + \exp\left[\frac{E_\Gamma - \zeta}{k_B T} \right]}$$

$$\times \frac{E_\Gamma}{k_B T} \left(1 + \frac{E_\Gamma / k_B T}{E_G^* / k_B T}\right)^{\frac{1}{2}} \left(1 + 2\frac{E_\Gamma / k_B T}{E_G^* / k_B T}\right) d\left(\frac{E_\Gamma}{k_B T}\right) \tag{1.24}$$

where h is the Planck constant and k_B is the Boltzmann constant. By defining new variables $y = E_\Gamma / k_B T$, $\eta_\Gamma = \zeta / k_B T$ and $\beta = k_B T / E_G^*$,

we have

$$n_\Gamma = \frac{4}{\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2} \right)^{3/2} \int_0^\infty f_o(y, \eta_\Gamma) \left[y + \beta y^2 \right]^{\frac{1}{2}} (1 + 2\beta y) dy$$

$$= \frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2} \right)^{3/2} \int_0^\infty f_o(y, \eta_\Gamma) d \left[y + \beta y^2 \right]^{3/2} \qquad (1.25)$$

Integration by parts gives

$$n_\Gamma = \frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2} \right)^{3/2} \left[f_o(y, \eta_\Gamma) \left[y + \beta y^2 \right]^{3/2} \Big|_0^\infty \right.$$

$$\left. - \int_0^\infty \left(\frac{\partial f_o}{\partial y} \right) (y + \beta y^2)^{3/2} \, dy \right] . \qquad (1.26)$$

Since the first term vanishes for both limits, we have

$$n_\Gamma = \frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2} \right)^{3/2} {}_oL_o^{3/2} (\eta_\Gamma, \beta) \qquad (1.27)$$

where ζ is the Fermi level, $\eta_\Gamma = \zeta / k_B T$ is the reduced Fermi level

and $\beta = k_B T/E_G^*$ and ${}^{m}L_{k}^{n}(\eta,\beta)$ is a generalized Fermi-Dirac integral[14]

$$ {}^{m}L_{k}^{n}(\eta,\beta) = \int_0^\infty \left(-\frac{\partial f_o(y,\eta)}{\partial y}\right) y^m (y + \beta y^2)^n (1 + 2\beta y)^k dy . \quad (1.28) $$

In general, the generalized Fermi-Dirac integrals can not be solved analytically, and therefore, we shall evaluate the function ${}^{o}L_{o}^{3/2}(\eta_\Gamma, \beta)$ numerically. We shall discuss this type of function in the next chapter.

Another application of (1.20) is to obtain an energy dependent expression for m^*. By substituting from (1.20) into (1.7), we obtain

$$ m^* = m_\Gamma\left(1 + 2\,\frac{E_\Gamma}{E_G^*}\right) . \quad (1.29) $$

1.3 The Electrical Conductivity

The result (1.9) in Section 1.1 for the electrical conductivity involves the relaxation time τ which is assumed to exist. It is the purpose of this section to discuss the existence of a relaxation time for the scattering mechanisms in a polar semiconductor such as InSb in the temperature range from 77 K to

300 K. The two dominant scattering mechanisms are the impurity scattering and the polar scattering. The impurity scattering dominates at low temperatures (0 K - 100 K) and the polar scattering at high temperatures (200 K - 500 K). We shall treat the two cases separately.

1.3a The Low Temperature Case (Impurity Scattering)

The scattering mechanism predominant throughout the temperature range of 0 K - 100 K is the scattering due to the ionized impurities. Since the energy emitted or absorbed by an electron in a collision with ionized impurities (bound positive atoms for donors) is small compared with the initial energy of the electron, the relaxation time approximation is valid. According to Barrie's result for electrons in a nonparabolic band scattered by ionized impurities, the relaxation time τ_i is[15]

$$\tau_i = \frac{\hbar\varepsilon^2}{2\pi e^4 N} \left[\ln\left(1 + \frac{4k^2}{q^2}\right) - \frac{4k^2}{q^2 + 4k^2} \right]^{-1} k^2 \frac{dE}{dk} \qquad (1.30)$$

where ε is the dielectric constant of the material under consideration, N is the concentration of scattering centres which will be equal to the conduction electron concentration n_Γ in a non-compensated n-type extrinsic sample (i.e. $N = n_\Gamma$), and q is the

the screening constant in the perturbing impurity potential $V(r) = \frac{e^2}{\varepsilon r} \exp(-qr)$. The quantity $\left[\ln(1 + \frac{4k^2}{q^2}) - \frac{4k^2}{q^2+4k^2}\right]^{-1}$ is a slowly varying function of k so that it may be replaced by a constant γ in the integral involved in (1.9).

Now, the relaxation time τ_i is of the form

$$\tau_i = \frac{\gamma\hbar\varepsilon^2}{2\pi e^4 n_\Gamma} k^2 \frac{dE}{dk} . \qquad (1.31)$$

To obtain the energy dependent τ_i for the conduction electrons, we substitute (1.20) and (1.27) into (1.31):

$$\tau_i = \frac{\gamma\hbar\varepsilon^2}{2\pi e^4 n_\Gamma} \left\{ \frac{2m_\Gamma E_G^*}{\hbar^2} \left[\frac{E_\Gamma}{E_G^*}\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right] \right\} \left\{ \frac{2\hbar\sqrt{E_G^*}}{\sqrt{2m_\Gamma}} \frac{\left[\frac{E_\Gamma}{E_G^*}\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^{1/2}}{\left(1 + 2\frac{E_\Gamma}{E_G^*}\right)} \right\}$$

$$= \frac{3\gamma\pi\hbar^3\varepsilon^2}{2e^4 m_\Gamma (k_B T)^{3/2}\, {}^{o}L_o^{3/2}(n_\Gamma, \beta)} \frac{\left[E_\Gamma\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^{1/2}}{\left(1 + 2\frac{E_\Gamma}{E_G^*}\right)} . \qquad (1.32)$$

Substituting (1.20), (1.21), (1.29) and (1.32) into (1.9), we obtain the expression for the electrical conductivity σ_L at

low temperatures,

$$\sigma_L = \frac{\hbar^2 e^2}{3\pi^2} \int_0^\infty \left(-\frac{\partial f_o}{\partial E}\right) \left\{ \frac{3\gamma\pi\hbar^3 \varepsilon^2}{2e^4 m_\Gamma (k_B T)^{3/2}\, {}^oL_o^{3/2}(\eta_\Gamma, \beta)} \frac{\left[E_\Gamma\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^{1/2}}{\left(1 + 2\frac{E_\Gamma}{E_G^*}\right)} \right\}$$

$$\times \left\{ \frac{1}{m_\Gamma^2\left(1 + 2\frac{E_\Gamma}{E_G^*}\right)^2} \right\} \left\{ \frac{4m_\Gamma^2}{\hbar^4}\left[E_\Gamma\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^2 \right\} \left\{ \frac{2^{1/2} m_\Gamma^{1/2}}{2\pi\hbar} \frac{\left(1 + 2\frac{E_\Gamma}{E_G^*}\right)}{\left[E_\Gamma\left(1 + \frac{E_\Gamma}{E_G^*}\right)\right]^{1/2}} dE_\Gamma \right\}$$

$$= \frac{2^{1/2}\gamma (k_B T)^{3/2} \varepsilon^2}{\pi e^2 m_\Gamma^{1/2}\, {}^oL_o^{3/2}(\eta_\Gamma, \beta)} \int_0^\infty \left(-\frac{\partial f_o}{\partial E}\right) \left[\frac{E_\Gamma}{k_B T}\left(1 + \frac{E_\Gamma/k_B T}{E_G^*/k_B T}\right)\right]^3$$

$$\times \left(1 + 2\frac{E_\Gamma/k_B T}{E_G^*/k_B T}\right)^{-2} d\frac{E_\Gamma}{k_B T} \quad . \tag{1.33}$$

Again, using the variables $y = \frac{E_\Gamma}{k_B T}$, $\eta_\Gamma = \frac{\zeta}{k_B T}$ and $\beta = \frac{k_B T}{E_G^*}$, we have

$$\sigma_L = \frac{2^{1/2}\gamma (k_B T)^{3/2}}{\pi e^2} \frac{\varepsilon^2}{m_\Gamma^{1/2}} \frac{{}^oL_{-2}^3(\eta_\Gamma, \beta)}{{}^oL_o^{3/2}(\eta_\Gamma, \beta)} \quad . \tag{1.34}$$

1.3b The High Temperature Case (Polar Scattering)

At temperature above 200 K, the polar scattering dominates the transport phenomena in InSb. Ehrenreich[1] calculated the electrical conductivity of InSb due to polar scattering by using the variational formulation which is the proper procedure to solve the Boltzmann equation since it is questionable to define a relaxation time for polar scattering at temperatures near or below the Debye temperature Θ of the material (for InSb, Θ = 290 K). However Ehrenreich's treatment becomes too complex for a discussion of the pressure effects. For simplicity, we shall assume a relaxation time τ_p exists in the temperature range of 200 K - 300 K and compare the pressure dependent electrical conductivity with the experimental data. According to Frohlich,[16] the relaxation time τ_p for this temperature range is given by

$$\tau_p = \frac{2^{\frac{1}{2}}\hbar\nu\left(\exp\frac{h\nu}{k_B T} - 1\right)M\upsilon_a E^{\frac{1}{2}}}{e^2(e^*)^2(m^*)^{\frac{1}{2}}} \qquad (1.35)$$

where ν is the optical oscillation frequency of the ions, M is the reduced mass of the ions, e is the free electron charge, e^* is the effective charge[1] and υ_a is the volume of the unit cell.

For conduction electrons in InSb, the relaxation time τ_p is obtained by substituting (1.29) into (1.35), i.e.

$$\tau_p = \frac{2^{\frac{1}{2}}\hbar\nu(\exp\frac{h\nu}{k_BT} - 1)M\upsilon_a E_\Gamma^{\frac{1}{2}}}{e^2(e^*)^2 m_\Gamma^{\frac{1}{2}}(1+2\frac{E_\Gamma}{E_G^*})^{\frac{1}{2}}} \quad . \tag{1.36}$$

Similar to the calculation in Section 3.1, by substituting (1.20), (1.29) and (1.36) into (1.9), we obtain the expression for the electrical conductivity σ_H at high temperatures

$$\sigma_H = \frac{\hbar^2 e^2}{3\pi^2}\int_0^\infty (-\frac{\partial f_o}{\partial E_\Gamma})\left\{\frac{2^{\frac{1}{2}}M\hbar\nu(\exp\frac{h\nu}{k_BT} - 1)\upsilon_a E_\Gamma^{\frac{1}{2}}}{e^2(e^*)^2 m_\Gamma^{\frac{1}{2}}(1+2\frac{E_\Gamma}{E_G^*})^{\frac{1}{2}}}\right\}\left\{\frac{1}{m_\Gamma^2(1+2\frac{E_\Gamma}{E_G^*})^2}\right\}$$

$$\times\left\{\frac{4m_\Gamma^2}{\hbar^4}\left[E_\Gamma(1+\frac{E_\Gamma}{E_G^*})\right]^2\right\}\left\{\frac{2^{\frac{1}{2}}m_\Gamma^{\frac{1}{2}}}{2\hbar}\frac{(1+2\frac{E_\Gamma}{E_G^*})}{E_\Gamma(1+\frac{E_\Gamma}{E_G^*})^{\frac{1}{2}}}\,dE_\Gamma\right\} . \tag{1.37}$$

Again, using the variables $y = \frac{E_\Gamma}{k_BT}$, $\eta_\Gamma = \frac{\zeta}{k_BT}$ and $\beta = \frac{k_BT}{E_G^*}$, we obtain

$$\sigma_H = \left[\frac{4M\nu(k_BT)^2(\exp\frac{h\nu}{k_BT} - 1)}{3\pi^2\hbar^2}\right]\frac{\upsilon_a}{(e^*)^2}\,{}^{\frac{1}{2}}L_{-\frac{3}{2}}^{\frac{3}{2}}(\eta_\Gamma, \beta) \quad . \tag{1.38}$$

CHAPTER 2 The Hydrostatic Pressure Effects

There are many experiments,[6,7] which indicate that the energy band structure of InSb changes significantly due to hydrostatic pressure change and consequently the energy differences between the extrema of various bands are pressure sensitive. In this chapter, we are going to determine the dependence of the parameters which appear in (1.34) and (1.38) upon these energy differences so as to obtain the pressure dependence of the electrical conductivity.

2.1 Determination of the Fermi Level

Since the generalized Fermi-Dirac integrals ${}^{m}L_{k}^{n}(\eta, \beta)$ which appear both in (1.34) and (1.38) are functions of the reduced Fermi level, $\eta_\Gamma = \zeta/k_B T$, we need to determine the Fermi level ζ corresponding to the carrier concentrations in thermal equilibrium.

2.1a The Low Temperature Case

At low temperatures, essentially all the electrons in the first conduction band are excited from the donor impurity level. Therefore, for the low temperature range, we shall

determine the Fermi level by equating the electron concentration in the first conduction band to the ionized donor concentration of the impurity level. If we denote n_I as the ionized donor concentration of an impurity level E_I below the bottom of the first conduction band; then, from Fermi-Dirac statistics, n_I is given by

$$n_I = (1 - f_o(E_I))\, N_D$$

$$= \frac{N_D}{1 + \exp\left(\frac{E_I + \zeta}{k_B T}\right)} \qquad (2.1)$$

where N_D is the total impurity density (10^{14} cm^{-3} in the sample experimentally studied[9]). The impurity energy level E_I is determined by using the hydrogen-like atom approach,[12] assuming that we have a single monovalent donor sample. E_I is then given by

$$E_I = \frac{e^4 m_\Gamma}{2\hbar^2 \varepsilon^2} \quad . \qquad (2.2)$$

We shall discuss in the next section the temperature and pressure dependence of E_I which arises from the temperature and pressure dependence of both the band minimum effective mass m_Γ and the static dielectric constant ε.

Since we assume that all conduction electrons are excited from the impurity level at low temperatures (i.e. $n_\Gamma = n_I$), we have from (1.27) and (2.1)

$$\frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2} \right)^{3/2} {}^{o}L_{o}^{3/2} (n_\Gamma, \beta)$$

$$- \frac{N_D}{1 + \exp \left(\frac{E_I}{k_B T} + n_\Gamma \right)} = 0 . \qquad (2.3)$$

This relation can be used to determine the Fermi level.

2.1b The High Temperature Case

At high temperatures (200 K - 300 K), InSb behaves nearly as an intrinsic semiconductor and the conduction electrons are mainly contributed from the various valence bands. To determine the Fermi level in thermal equilibrium at high temperatures, we need to know the band structure of InSb to obtain the carrier concentrations in various bands.

The band structure of InSb was calculated by Kane[8] using the $\underset{\sim}{k} \cdot \underset{\sim}{p}$ perturbation approach. Since InSb has a narrow forbidden energy gap, the structures of the first conduction band,

the light-hole valence band and the spin-orbit split-off band are determined by treating the mutual interactions of these three bands exactly, while the higher bands are treated by perturbation theory. The results from Kane's calculation are

$$
\begin{aligned}
E_{\Gamma} &= \frac{\hbar^2 k^2}{2m_o} + \tfrac{1}{2}\left[(E_G^{*2} + \frac{8}{3} P^2 k^2)^{\frac{1}{2}} - E_G^{*} \right] , \\
E_{v1} &= - \frac{\hbar^2 k^2}{2m_o} - E_G , \\
E_{v2} &= - \frac{\hbar^2 k^2}{2m_o} + \tfrac{1}{2}\left[- (E_G^{*2} + \frac{8}{3} P^2 k^2)^{\frac{1}{2}} - E_G^{*} \right]
\end{aligned}
\qquad (2.4)
$$

and

$$
E_{v3} = - (E_G + \Delta) - \frac{\hbar^2 k^2}{2m_o} - \frac{P^2 k^2}{3(E_G + \Delta)} .
$$

The symbols E_{Γ}, E_{v1}, E_{v2} and E_{v3} denote the energy of the first conduction band, the heavy-hole valence band, the light-hole valence band and the spin-orbit split-off valence band respectively. The parameters used in these results are m_o the mass of the free electron, E_G the forbidden band gap (for InSb, E_G = 0.23 eV at T = 0 K), E_G^{*} the effective mass energy gap which is assumed to affect the effective masses of the first conduction band and the light-hole valence band only[1], P the matrix element of the

'interband' interaction and Δ the spin-orbit splitting of the valence band. The value of P has been determined in (1.15). While Δ has not yet been determined experimentally, Kane assumed a value of 0.9 eV by combining the estimated values of the spin-orbit splitting of the atomic p-functions in the two different atoms, indium and antinomy.

From (2.4), the expressions for E_Γ and E_{v2} indicate the energy band structure of these two bands are nonparabolic. The degree of nonparabolicity is determined by the quantity P^2k^2 occuring in the second term of the expressions. The extrema of these two bands are both at k = 0. Since the effective masses are very small at these band extrema ($m_\Gamma(0,0) = 0.013\ m_o$ [13] and $m_{v2}(0,0) = 0.015\ m_o$ [8]), the curvature of each band is very large at k = 0. According to (2.4), the curvature decreases with increasing k and thus the energy departs from a parabolic band away from k = 0. The difference between the first conduction band and a standard parabolic band is shown in Fig. 2.1 The reason for considering the nonparabolicity of these two bands in transport properties arises from the fact that the densities of states of the occupied parts of the parabolic and of the proper nonparabolic band differ by a significant amount at room temperature so that one should not neglect it in the calculation of carrier concentration (H. Ehrenreich has discussed this problem and concluded that the difference involved at room temperature is more than 50% [1]).

The expression for the heavy-hole valence band in (2.4) is less satisfactory. Experimental evidence[17] indicates that the heavy-hole effective mass m_{v1} has a value of 0.4 m_o, rather than being equal to the free electron mass as in (2.4). Therefore we shall modify Kane's result by replacing m_o by $m_{v1} = 0.4\ m_o$, i.e.

$$E_{v1} = -\frac{\hbar^2 k^2}{2m_{v1}} - E_G . \tag{2.5}$$

In addition to the bands described by (2.4), many experiments suggest the existence of a higher conduction band E_L with $E_{\Gamma L} \equiv (E_L - E_\Gamma)_{min.} = 0.5$ eV at atmospheric pressure. This band is assumed to be parabolic with an effective mass $m_L = 0.5\ m_o$.[8,18] With this additional L - band taken into account, the entire band structure of InSb is given by

$$E_L = \frac{\hbar^2 k^2}{2m_L} + E_{\Gamma L} , \tag{2.6a}$$

$$E_\Gamma = \frac{\hbar^2 k^2}{2m_o} + \tfrac{1}{2}\left[(E_G^{*2} + \frac{8}{3} P^2 k^2)^{\frac{1}{2}} - E_G^* \right], \tag{2.6b}$$

$$E_{v1} = -\frac{\hbar^2 k^2}{2m_{v1}} - E_G , \tag{2.6c}$$

$$E_{v2} = -\frac{\hbar^2 k^2}{2m_o} + \tfrac{1}{2}\left[-(E_G^{*2} + \frac{8}{3} P^2 k^2)^{\frac{1}{2}} - E_G^* \right] \tag{2.6d}$$

and

$$E_{v3} = -(E_G + \Delta) - \frac{\hbar^2 k^2}{2m_o} - \frac{P^2 k^2}{3(E_G + \Delta)} . \tag{2.6e}$$

This is illustrated in Fig. 2.1.

The calculation of carrier concentrations in various bands is similar to that for the first conduction band in section 1.2. The equations (1.22) and (1.23) are again applied with the corresponding energy dependent wave number formulae derived from the band structure.

For the L - conduction band, (2.6a) gives

$$k = \frac{(2m_L)^{\frac{1}{2}}}{\hbar} (E_L - E_{\Gamma L})^{\frac{1}{2}} \qquad (2.7)$$

and thus the electron concentration in the L - conduction band will be given by

$$n_L = \int_{E_{\Gamma L}}^{\infty} f_o(E_L)\, g(E_L)\, dE_L$$

$$= \frac{4}{\pi^{\frac{1}{2}}} \left(\frac{2\pi m_L}{h^2}\right)^{3/2} \int_{E_{\Gamma L}}^{\infty} \frac{1}{1 + \exp\left(\frac{E_L - \zeta}{k_B T}\right)} (E_L - E_{\Gamma L})^{\frac{1}{2}}\, dE_L . \qquad (2.8)$$

Setting $y = \frac{E_L - E_{\Gamma L}}{k_B T}$ and $\eta_L = \frac{\zeta - E_{\Gamma L}}{k_B T}$, we have

$$n_L = 2 \left(\frac{2\pi m_L k_B T}{h^2}\right)^{3/2} \mathfrak{F}_{\frac{1}{2}}(\eta_L) \qquad (2.9)$$

where $\mathfrak{F}_j(\eta) \equiv \frac{2}{\pi^{\frac{1}{2}}} \int_0^\infty \frac{y^j}{1 + \exp(y - \eta)}\, dy$ is the Fermi-Dirac integral.[19] In InSb, $E_{\Gamma L}$ has a value of 0.5 eV while the main energy gap E_G = 0.23 eV at zero temperature. Since the Fermi level η is within the main gap, the quantity $\eta_L = (\zeta - E_{\Gamma L})/k_B T$ at room temperature is always a large negative number, so that by following Blakemore's arguement,[19] we make the approximation

$$\mathfrak{F}_{\frac{1}{2}}(\eta_L) \simeq \exp(\eta_L). \tag{2.10}$$

Thus (2.9) becomes

$$n_L = 2 \left(\frac{2\pi m_L k_B T}{h^2}\right)^{3/2} \exp(\eta_L). \tag{2.11}$$

For the heavy-hole valence band, (2.6c) gives

$$k = \pm \left(\frac{2m_{v1}}{h^2}\right)^{\frac{1}{2}} (- E_{v1} - E_G)^{\frac{1}{2}} \tag{2.12}$$

(Note that we shall choose the negative sign in this expression for k in order to obtain a real physical description for the hole concentration). By following the same approach as for the L - band except using the hole distribution function $[1 - f_o(E)]$, the hole concentration in the heavy-hole valence band is

$$p_{v1} = 2 \left(\frac{2\pi m_{v1} k_B T}{h^2}\right)^{3/2} \mathfrak{F}_{1/2}(\eta_{v1}) \tag{2.13}$$

where $\eta_{v1} = -\frac{(\zeta + E_G)}{k_B T}$. Since η_{v1} has a value close to zero room temperature, we approximate $\mathfrak{F}_{1/2}(\eta_{v1})$ as[19]

$$\mathfrak{F}_{1/2}(\eta_{v1}) \simeq \frac{\exp(\eta_{v1})}{1 + 0.27 \exp(\eta_{v1})} , \tag{2.14}$$

and thus (2.13) becomes

$$p_{v1} = 2 \left(\frac{2\pi m_{v1} k_B T}{h^2}\right)^{3/2} \frac{\exp(\eta_{v1})}{1 + 0.27 \exp(\eta_{v1})} . \tag{2.15}$$

The expression (2.6e) for the spin-orbit split-off valence band can be rewritten in a simple parabolic form

$$E_{v3} = -\frac{\hbar^2 k^2}{2m_{v3}} - (E_G + \Delta) , \tag{2.16}$$

by defining an effective mass $m_{v3} \equiv \hbar^2 \left(\frac{d^2 E_{v3}}{dk^2}\right)^{-1}$. From (2.6e), m_{v3} is given by

$$m_{v3} = \hbar^2 \left[\frac{\hbar^2}{m_o} - \frac{2P^2}{3(E_G + \Delta)}\right]^{-1} \tag{2.17}$$

and is approximately 0.115 m_o. Equation (2.16) gives the energy dependent k in this band as

$$k = - \left(\frac{2m_{v3}}{h^2}\right)^{\frac{1}{2}} - (E_{v3} + E_G + \Delta)^{\frac{1}{2}} . \qquad (2.18)$$

By following the same approach as for the L - band, the hole concentration in the spin-orbit valence band is

$$p_{v3} = 2 \left(\frac{2\pi m_{v3} k_B T}{h^2}\right)^{3/2} \exp(\eta_{v3}) \qquad (2.19)$$

where $\eta_{v3} = - \dfrac{(\zeta + E_G + \Delta)}{k_B T}$.

For the nonparabolic bands of InSb, we have already calculated the electron concentration in the first conduction band. The result for n_Γ is given by (1.27). A similar calculation can be applied to determine the hole concentration in the light-hole valence band and a result similar to (1.27) is obtained by approximating the upper limit E_2 in (1.22) by E_G^* instead of using the correct quantity E_G. This approximation is valid, since the number of electrons excited from the light-hole valence band is much smaller than that from the heavy-hole valence band. The hole concentration in the light-hole valence band so obtained is

$$p_{v2} = \frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_{v2} k_B T}{h^2}\right)^{3/2} {}_{o}L_{o}^{3/2}(\eta_{v2}, \beta) \qquad (2.20)$$

where $\eta_{v2} = -\frac{(\zeta + E_G^*)}{k_B T}$.

In general, especially in the temperature range where the intrinsic and extrinsic transitions are both important, the condition of electric neutrality of the crystal requires that the electron concentration in the conduction bands should be equal to the ionized donor concentration from the impurity level plus the hole concentration in the valence bands, i.e.

$$n_\Gamma + n_L = n_I + p_{v1} + p_{v2} + p_{v3} . \qquad (2.21)$$

Substituting (1.27), (2.1), (2.11), (2.15), (2.19) and (2.20) into (2.21), we obtain

$$\frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_\Gamma k_B T}{h^2}\right)^{3/2} {}_{o}L_{o}^{3/2}(\eta_\Gamma, \beta) + 2\left(\frac{2\pi m_L k_B T}{h^2}\right)^{3/2} \exp(\eta_L)$$

$$- \frac{N_D}{1 + \exp\left(\frac{E_I}{k_B T} + \eta_\Gamma\right)} + 2\left(\frac{2\pi m_{v1} k_B T}{h^2}\right)^{3/2} \frac{\exp(\eta_{v1})}{1 + 0.27\exp(\eta_{v1})}$$

$$+ \frac{8}{3\pi^{\frac{1}{2}}} \left(\frac{2\pi m_{v2} k_B T}{h^2}\right)^{3/2} {}_{o}L_{o}^{3/2}(\eta_{v2}, \beta)$$

$$+ 2\left(\frac{2\pi m_{v3} k_B T}{h^2}\right)^{3/2} \exp(\eta_{v3}) = 0 . \qquad (2.22)$$

The variables in (2.22) are the temperature T and the Fermi level ζ, therefore we can use (2.22) to determine the Fermi level at high temperatures.

2.2 Temperature and Pressure Dependent Parameters

2.2a The Energy Differences between Various Band Extrema

In semiconductors, a change in temperature will cause a change in the lattice constants due to thermal expansion as well as a change in the oscillation frequency of the ions associated with the variation of the specific heat. These two mechanisms contribute the total temperature induced change of the main energy gap E_G (the energy difference between the first conduction band and the first valence band), and the temperature coefficient $(\partial E_G/\partial T)_P$ has been determined to be -2.9×10^{-4} eV/K from the measurement of optical absorption in n-InSb.[20] However, it is only the change of the energy gap with temperature due to the lattice dilatation which will change the curvature near the first conduction band minimum (i.e. will change the band minimum effective mass m_Γ).[1] To eliminate the effect of the change in the oscillation frequency

of the ions with temperature, we have to use the effective mass energy gap E_G^* instead of E_G to calculate the change in m_Γ. Ehrenreich[1] calculated the temperature coefficient $(\partial E_G^*/\partial T)_P$ to be -0.96×10^{-4} eV/K.

Ehrenreich[1] assumed that the pressure coefficients of these two energy gaps are the same, i.e. $(\partial E_G/\partial P)_T = (\partial E_G^*/\partial P)_T$. Various values of $(\partial E_G/\partial P)_T$ have been reported from many experiments.[6,7] Most of the experimental values were obtained from electrical resistivity data with considerable theoretical uncertainty,[6,7] therefore we choose the value $(\partial E_G/\partial P)_T = 1.6 \times 10^{-2}$ eV/kbar which has been obtained from the optical measurement of the energy gap up to 30 kbar.[6]

If we assume a linear relation of the energy gaps with temperature and pressure which is, in fact, observed experimentally, then the temperature and pressure dependence of E_G and E_G^* can be written as

$$E_G(T,P) = E_G(0,0) + \left(\frac{\partial E_G}{\partial T}\right)_P T + \left(\frac{\partial E_G}{\partial P}\right)_T P \qquad (2.23)$$

and

$$E_G^*(T,P) = E_G(0,0) + \left(\frac{\partial E_G^*}{\partial T}\right)_P T + \left(\frac{\partial E_G}{\partial P}\right)_T P \qquad (2.24)$$

where $E_G(0,0) = 0.24855$ eV is the value for E_G at zero temperature and at atmospheric pressure extrapolated from the high temperature

region of the E_G vs T curve[20]. This value should be distinguished from the exact value E_{GO} = 0.23 eV at zero temperature, since the temperature dependence of the energy gap is nonlinear in the low temperature range, 0 K - 100 K.

The magnitude and pressure dependence of $E_{\Gamma L}$ are not well known; however in analogy with other Ge-type semiconductors and with some theoretical and experimental support, it is thought that

$$E_{\Gamma L}(P) = E_{\Gamma L}(0) + \left(\frac{\partial E_{\Gamma L}}{\partial P}\right)_T P \qquad (2.25)$$

where $E_{\Gamma L}(0)$ = 0.5 eV[8,18] and $(\partial E_{\Gamma L}/\partial P)_T$ = - 10^{-2} eV/kbar.[9]

2.2b The Effective Masses

The conduction band minimum effective mass m_Γ is related to the effective mass energy gap E_G^* and the interband interaction matrix element by (1.15). Ehrenreich assumed that this matrix element is weakly temperature and pressure dependent.[1] With a further assumption that the variation of the ratio of the effective mass and the free electron mass μ is small compared with unity, it follows that $(1 - \mu) \approx$ const., and then (1.15) gives the relation

$$\frac{E_G^*(T,P)}{m_\Gamma(T,P)} = \text{const.} \quad . \qquad (2.26)$$

Thus the temperature and pressure dependence of m_Γ is

$$m_\Gamma\ (T,P) = m_\Gamma(0,0)\ \frac{E_G^*\ (T,P)}{E_G^*\ (0,0)}$$

$$= m_\Gamma(0,0)\left[1 + \frac{1}{E_G(0,0)}\ (\frac{\partial E_G^*}{\partial T})_P\ T + \frac{1}{E_G(0,0)}\ (\frac{\partial E_G}{\partial P})_T\ P\right] \tag{2.27}$$

where $m_\Gamma(0,0) = 0.013\ m_o$ is the band minimum effective mass at zero temperature and atmospheric pressure.

The temperature and pressure dependence of m_{v2} is similar to that of m_Γ and has the form

$$m_{v2}(T,P) = m_{v2}(0,0)\left[1 + \frac{1}{E_G(0,0)}(\frac{\partial E_G^*}{\partial T})_P T + \frac{1}{E_G(0,0)}\ (\frac{\partial E_G}{\partial P})_T\ P\right] \tag{2.28}$$

where $m_{v2}\ (0,0) = 0.015\ m_o$ is the value for m_{v2} at zero temperature and atmospheric pressure.

2.2c The Static Dielectric Constant

We write the static dielectric constant as a sum of the contributions from the lattice polarization ε_{lat} and the electronic polarization ε_{el}, i.e.

$$\varepsilon = \varepsilon_{lat} + \varepsilon_{el}. \tag{2.29}$$

To derive the pressure dependence of ε, we first assume that the variation of ε_{lat} due to pressure is negligible. This assumption may be reasonable since $\varepsilon_{lat} = 2.2$ [21] is small compared with $\varepsilon_{el} = 15.7$ [22] at atmospheric pressure so that any small change in ε_{lat} will not be significant in the total change of ε. Therefore the pressure dependence of ε can be derived solely from the variation of ε_{el} due to pressure.

The Penn model[23] assumes an isotropic free-electron energy band throughout $\underset{\sim}{k}$ - space except near the Fermi surface where it has a gap E_p, the Penn gap. The electronic dielectric constant in this model is expressed as

$$\varepsilon_{el} = 1 + \left(\frac{\hbar\omega_p}{E_p} \right)^2 \tag{2.30}$$

where ω_p is the plasma frequency associated with the valence electrons.

Since the plasma frequency ω_p relates to the valence electron density $N = N_T/V$ (N_T is the total number of valence electrons and V is the volume of the crystal) by

$$\omega_p^2 = \frac{4\pi e^2 N}{m} \quad , \tag{2.31}$$

also the pressure dependence of N is given by

$$N(P) = N(0)\ (\ 1 + \kappa P) \tag{2.32}$$

where N(0) is the density at atmospheric pressure and $\kappa \equiv -\frac{1}{V}(\frac{dV}{dP})_T$ is the compressibility. We can find the pressure dependence of ω_p by substituting (2.32) into (2.31), i.e.

$$\omega_p^2(P) = \omega_p^2(0)\ (1 + \kappa P) \tag{2.33}$$

where $\omega_p(0)$ is the plasma frequency at atmospheric pressure.

The Penn gap E_p is also pressure dependent. Tsay et al.[24] assumed that E_p could be identified as the energy of the transition $\Sigma_{2,v} \rightarrow \Sigma_{3,c}$ based on the theoretical interpretation of the Penn model by Heine and Jones and the experimental optical spectrum. With this identification, E_p has a value of 3.7 eV at atmospheric pressure and a calculated pressure coefficient $(\partial E_p/\partial P)_T$ of 9.2×10^{-3} eV/kbar[24]. In basic agreement

with the optical results of Zallen and Paul[25] which indicate the $\Sigma_{2,v} \rightarrow \Sigma_{3,c}$ transition has a zero pressure value of 4.1 eV and a pressure derivative of 5.8×10^{-3} eV/kbar. We shall use the theoretical result and write the pressure dependence of E_p as

$$E_p(P) = E_p(0)\left[1 + \frac{1}{E_p(0)}\left(\frac{\partial E_p}{\partial P}\right)_T P\right] \tag{2.34}$$

Finally, the pressure dependence of the static dielectric constant ε is obtained from (2.29), (2.30), (2.33) and (2.34) as

$$\varepsilon(P) \simeq \varepsilon_{lat}(0) + 1 + \frac{\hbar^2\omega_p^2(0)}{E_p^2(0)}\left[1 + \kappa P\right] \times \left[1 + \frac{1}{E_p(0)}\left(\frac{\partial E_p}{\partial P}\right)_T P\right]^{-2} . \tag{2.35}$$

2.2d The Effective Charge

The effective charge is calculated by Ehrenreich[1] to be

$$e^{*2} = \frac{M\nu^2 v_a}{4\pi}\left(\frac{1}{\varepsilon_{el}} - \frac{1}{\varepsilon}\right) . \tag{2.36}$$

We shall neglect any pressure dependence of ν. Therefore the pressure dependence of the parameter (υ_a/e^{*2}) which appears in (1.38) arises from the term $(\varepsilon_{el}^{-1} - \varepsilon^{-1})$. From the assumptions made in Section 2.2c $(\varepsilon_{el}^{-1} - \varepsilon^{-1})$ is a very slowly varying function of pressure. Therefore we shall neglect the pressure dependence of (υ_a/e^{*2}).

2.2e The Generalized Fermi-Dirac Integrals

In Chapter 1, Section 1.2, it has been stated that the generalized Fermi-Dirac integrals could not be solved analytically. The functions ${}^{o}L_{o}^{3/2}(\eta_\Gamma,\beta)$, ${}^{o}L_{-2}^{3}(\eta_\Gamma, \beta)$ and ${}^{\frac{1}{2}}L_{-3/2}^{3/2}(\eta_\Gamma, \beta)$ in (1.34) and (1.38) depend upon temperature and pressure. We shall determine the effects of variation of these functions upon the electrical conductivity by direct numerical analysis at various temperatures and pressures. The variables η_Γ and β can be determined for a given temperature and pressure. To determine η_Γ and β, we use the equation (2.3) (for the low temperature case) or (2.22) (for the high temperature case) accompanied with the temperature and pressure dependent parameters expressed by (2.2) (2.23), (2.24), (2.25), (2.27), (2.28) and (2.35).

CHAPTER 3 Calculations and Results

3.1 The Pressure Dependent Electrical Conductivity at Low Temperature

Equation (1.34) has been used to calculated the pressure dependent electrical conductivity $\sigma_L(P)$ of n-type InSb at 81 K up to 10 kbar by substituting the temperature and pressure effects on the effective mass $m_\Gamma(T,P)$ from (2.27) and on the static dielectric constant $\varepsilon(P)$ from (2.35) and by following the procedure indicated for calculating the generalized Fermi-Dirac integrals ${}^oL_o^{3/2}(T,P)$ and ${}^oL_{-2}^{3}(T,P)$. The parameter γ in (1.34) has been chosen so that the calculated value of $\sigma_L(P)$ is in agreement with the measured value at 0.2 kbar.

To show the various contributions from the pressure dependent parameters of the electrical conductivity $\sigma_L(P)$, the calculated values of $\varepsilon(P)$, $m_\Gamma(P)$, ${}^oL_{-2}^{3}(P)/{}^oL_o^{3/2}(P)$ and $\sigma_L(P)/\sigma_L(0.2)$ at various pressures are shown in Table 3.1. The variation of the electrical conductivity $\sigma_L(P)$ as a function of pressure is compared with the experimental data[9] in Fig. 3.1. A good agreement with experiment is obtained for pressures up to

approximately 5 kbar. Progressive departure between the calculated and the observed values occurs for higher pressures.

3.2 The Pressure Dependent Electrical Conductivity at High Temperatures

Equation (1.38) has been used to calculate the pressure dependent electrical conductivity $\sigma_H(P)$ of n-type InSb at 290 K up to 10 kbar. Following the discussion in Section 2.2d, the only pressure dependent parameter is the generalized Fermi-Dirac integral ${}^{1/2}L^{3/2}_{-3/2}(P)$ which includes the variation of the conduction electron concentration and of the electron mobility due to pressure. The variation of the conduction electron concentration due to pressure is shown in Table 3.2. The pressure dependent concentration is in excellent agreement with the Hall measurement of the intrinsic carrier concentration[25]. The calculated electrical conductivity $\sigma_H(P)$ is compared with the experimental data[9] in Fig. 3.2. The theoretical results indicate a nearly linear relation between $\log \sigma_H(P)$ and P with $\log \sigma_H(P) = \log \sigma_H(P_o) + bP$ where b has a value of - 0.145 while the experimental results give a nonlinear relation, $\log \sigma_H(P) = \log \sigma_H(P_o) + b'P + c'P$ where $b' = -0.148$ and $c' = 0.0022$.

CHAPTER 4 Discussion and Conclusions

4.1 The Pressure Dependent Electrical Conductivity at Low Temperatures

The pressure dependent electrical conductivity for n-InSb at 81 K has been calculated by assuming the dominant mechanism for scattering of electrons to be ionized impurities. At low temperatures such as 81 K, it is known that the mobility is dominated by ionized impurity scattering in highly degenerated samples ($N_D > 10^{17}$ cm^{-3}) at atmospheric pressure[4]. Other experiments[27] indicate that at this temperature, impurity scattering dominates for samples with lower impurity concentrations down to at least 10^{15} cm^{-3}. For an undoped sample with $N_D = 10^{14}$ cm^{-3}, our calculation, in which no approximation is made for degeneracy, has a good agreement with experiment for pressures up to 5 kbar. Therefore, we do believe that the ionized impurity scattering is the only important mechanism at low temperatures.

In determining the impurity energy level E_I, we use the hydrogen-like atom approach, assuming that we have a single monovalent donor sample. It is the simplest method of calculating E_I which may oversimplify the problem of determining the Fermi level. In fact, the undoped sample which was used in the experiment may contain different types of impurities. There is no guarantee that

all impurities are single monovalent atoms. If part of impurities are multivalent atoms, instead of one single impurity energy level, there will be additional levels which are deeper in the forbiden energy gap. In this case, a decrease in electrical conductivity at higher pressures may arise from the decrease in the ionized donor concentration associated with the pressure dependence of these additional impurity energy levels. The simplification of our impurity model may explain the deviation between the calculated and the observed electrical conductivity which occurs at higher pressures.

In our model, we also exclude the possibility that the impurity atoms overlap with one another. Incousion of the overlap would lead to lowering of the binding energy of the donors. However at T = 81 K, all electrons are ionized even when overlap effects are neglected. Therefore we did not take the overlap effects into account in our calculation.

4.2 The Pressure Dependent Electrical Conductivity at High Temperatures

The pressure dependent electrical conductivity for n-InSb at 290 K has been calculated by assuming that a relaxation time exists in the polar scattering process. The theoretical result gives an under-estimate of σ at 290 K for high pressures.

Indeed, the theory does not include the nonlinear pressure effect of log σ_H (P) which is observed in experiment. At 290 K, the fact that electron mobility is dominated by the polar scattering has been already verified by Ehrenreich[1] at atmospheric pressure. Since our calculated results for the conduction electron concentration are in excellent agreement with experiment, the linear dependence of the energy differences between the various band extrema may be considered as a reasonable assumption. The absence of nonlinear pressure dependence of log σ_H (P) in our theory possibly may arise from the improper relaxation time assumption for the polar scattering process. This suggests that we should solve the Boltzmann equation by using the variational formulation to obtain the expression for the electrical conductivity.[1] Solving the Boltzmann equation without the relaxation time assumption is highly numerical. Therefore, unless this calculation is made, it is not known whether the improper relaxation time assumption would cause the under-estimate of the electrical conductivity at high pressures.

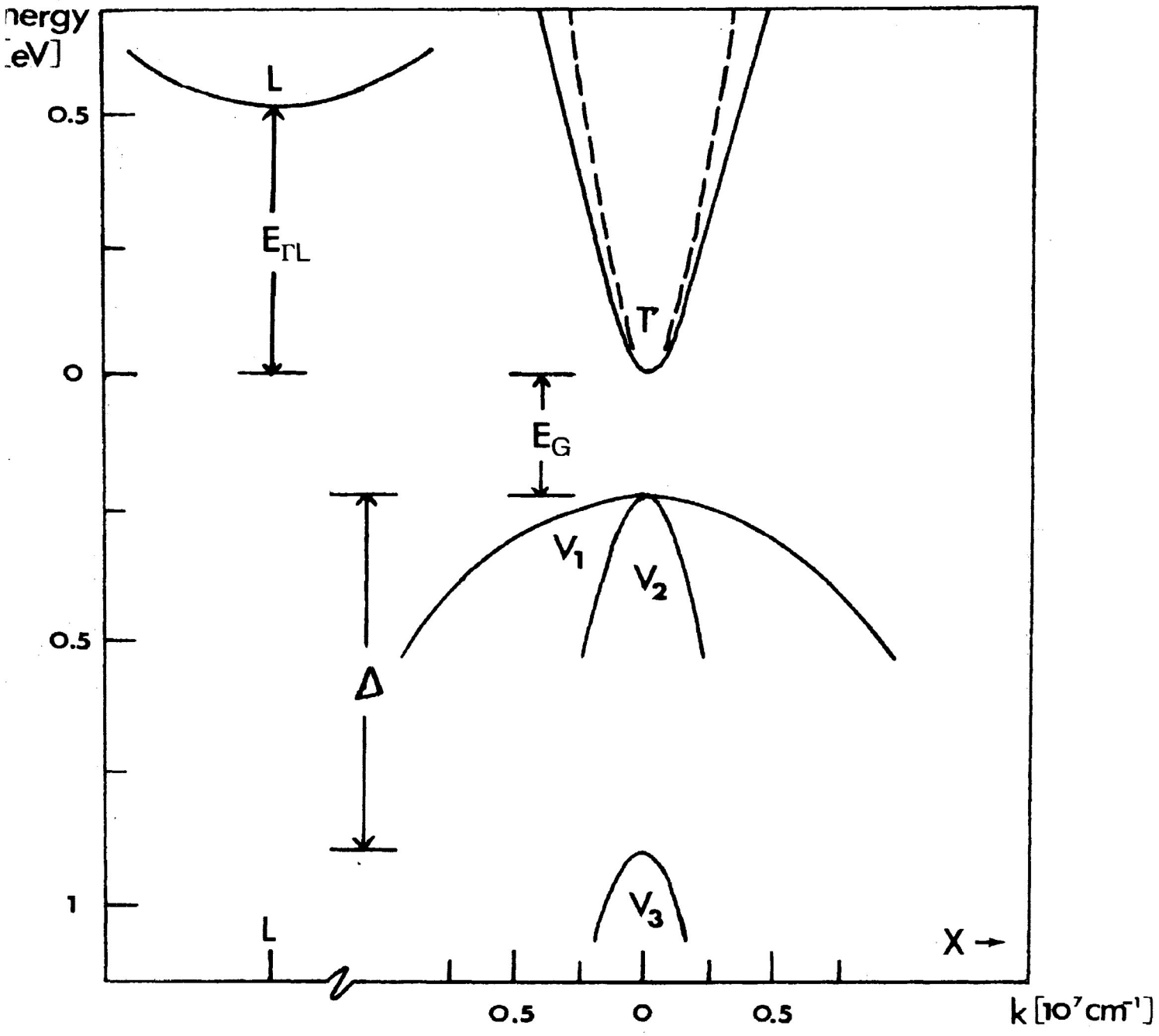

FIGURE 2.1 The Band Structure of InSb.

------- The shape of a parabolic conduction band with $m_\Gamma = 0.013\ m_o$ at k = 0.

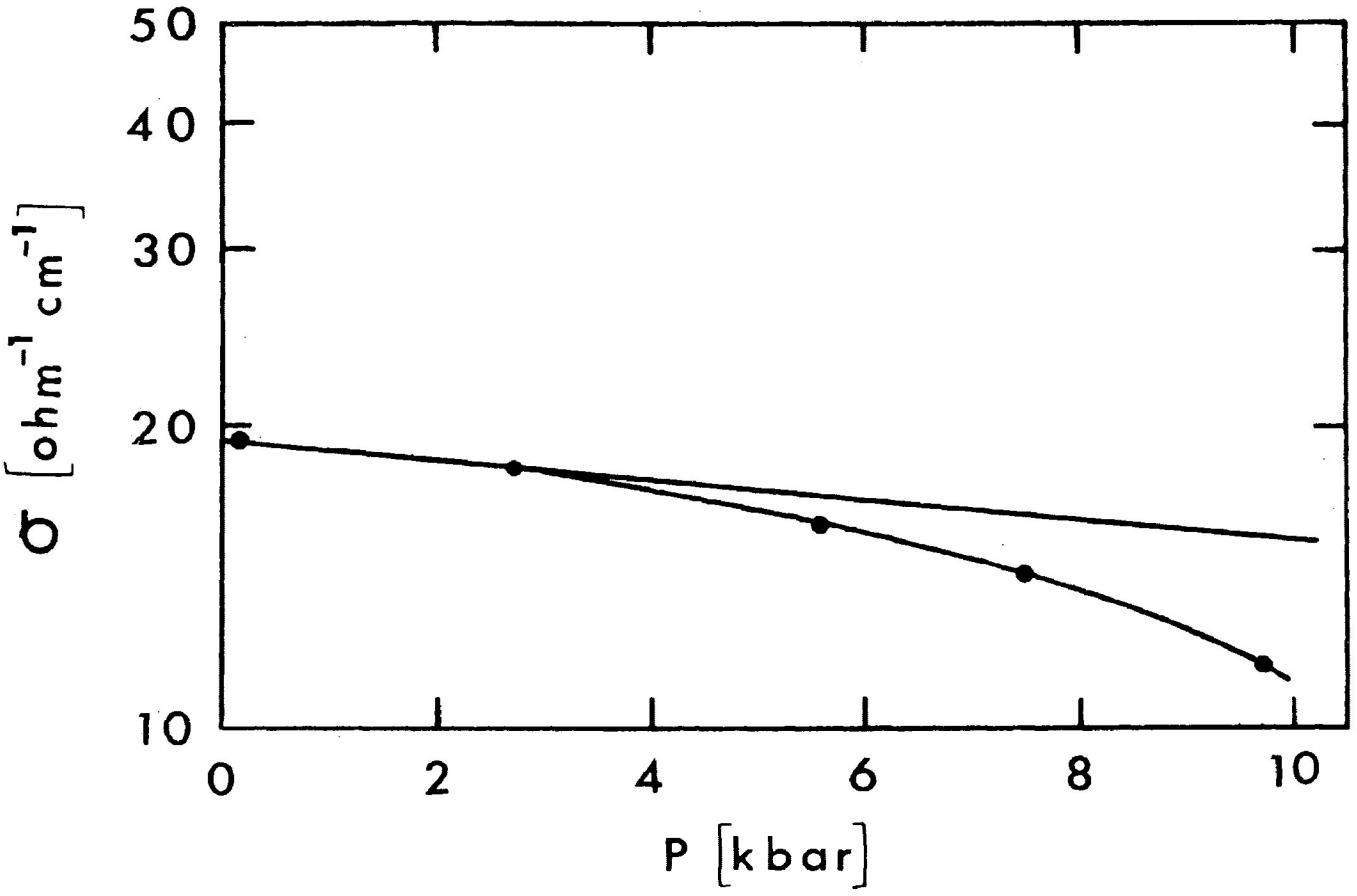

FIGURE 3.1 The pressure dependent electrical conductivity of n-type InSb ($N_D = 10^{14}$ cm^{-3}) at 81 K.

——— The theoretical result.

●—●—●—● The experimental result.

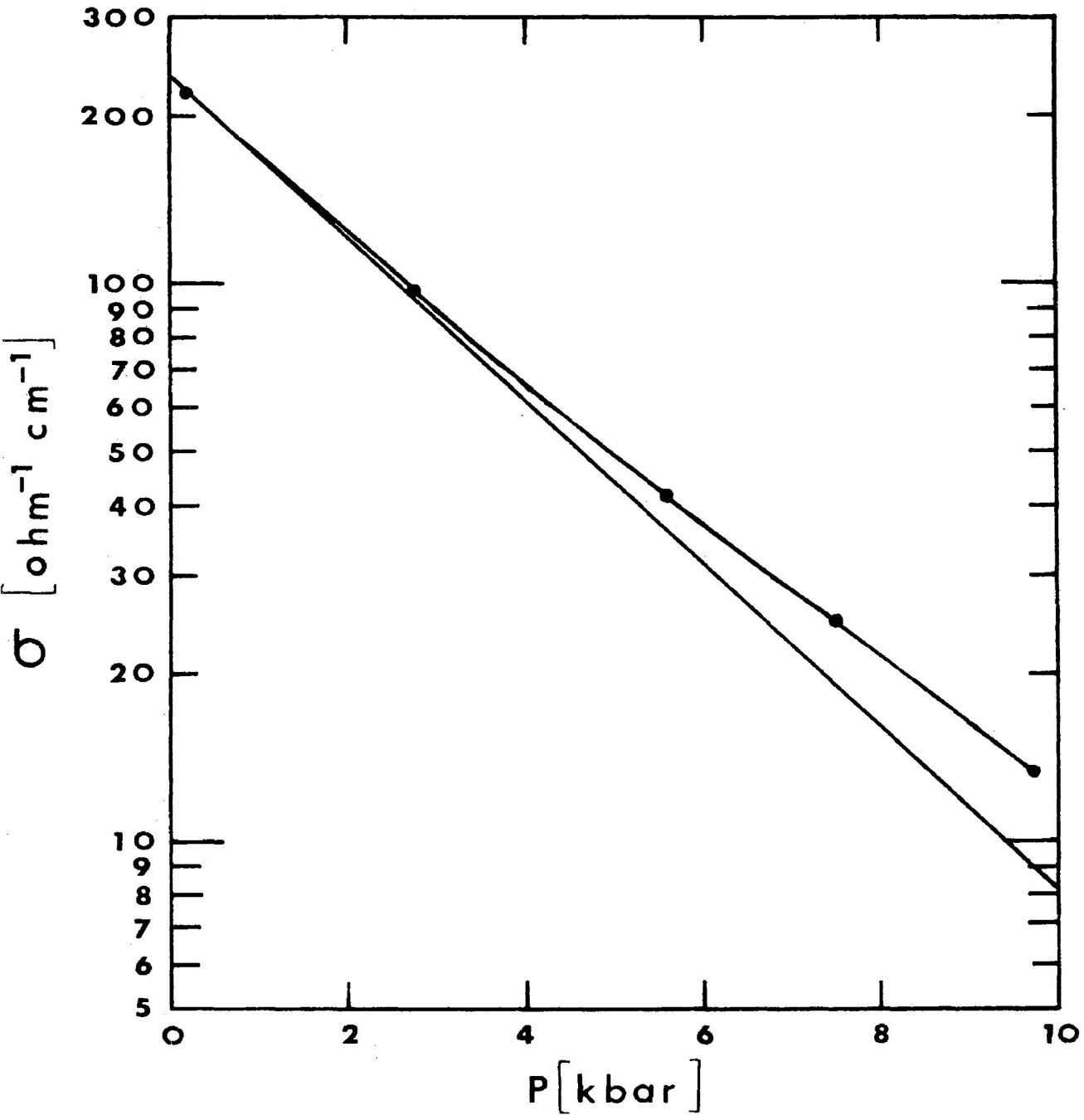

FIGURE 3.2 The pressure dependent electrical conductivity of n–type InSb ($N_D = 10^{14}$ cm^{-3}) at 290 K.

——— The theoretical result.

●——●——● The experimental result.

P (kbar)	ϵ	m_Γ (10^{-28} gm)	${}^{o}L_{-2}^{3}/{}^{o}L_{o}^{3/2}$	$\sigma_L(P)/\sigma_L(0.2)$
0	17.9	0.1147	3.7517	1.0057
0.2	17.89	0.1162	3.7585	1.0
1	17.86	0.1223	3.7873	0.9787
2	17.82	0.13	3.8216	0.9537
3	17.78	0.1376	3.8521	0.9304
4	17.74	0.1452	3.8811	0.9085
5	17.7	0.1528	3.9061	0.8867
6	17.66	0.1604	3.9304	0.8675
7	17.62	0.1681	3.9517	0.8477
8	17.58	0.1757	3.9728	0.8300
9	17.54	0.1833	3.9886	0.8124
10	17.5	0.1909	4.0073	0.7957

TABLE 3.1 Calculated values of the static dielectric constant ϵ, the effective mass m_Γ, the parameter ${}^{o}L_{-2}^{3}/{}^{o}L_{o}^{3/2}$, and the resulting relative conductivity at various pressures at 81 K.

P (k b a r)	n_Γ (10^{-16} cm^{-3})	p_{V_2} (10^{-13} cm^{-3})	η	β
0	1.858	1.610	-0.722	0.1132
0.2	1.765	1.554	-0.8	0.116
1	1.431	1.342	-1.1	0.1056
2	1.095	1.108	-1.47	0.09887
3	0.8338	0.9047	-1.83	0.09298
4	0.6323	0.7333	-2.19	0.08776
5	0.4782	0.5901	-2.55	0.08309
6	0.361	0.4717	-2.9	0.07889
7	0.2724	0.3745	-3.25	0.0751
8	0.2053	0.2960	-3.596	0.07165
9	0.1549	0.2323	-3.94	0.06851
10	0.117	0.1812	-4.27	0.06563

TABLE 3.2 The calculated values of the conduction electron concentration n_Γ, the light-hole concentration n_{v2}, the reduced Fermi level η_Γ and $\beta = k_B T / E_G^*$ at various pressures at 290 K.

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